CHEM 4616: Homework #8

Corresponds to the quiz to be given in class on Thursday, April 3rd, 2008

Chang, Chapter 17: Problems 32, 34-39

17.32

$\nu_L - \nu^\circ = 240\ Hz \qquad \nu^\circ = 60\ MHz$

$$\delta = \frac{\nu_L - \nu^\circ}{\nu^\circ} \times 10^6 = \boxed{4.0\ ppm}$$

17.34 $\quad \nu_L = \dfrac{\gamma B}{2\pi} \rightarrow B = \dfrac{2\pi \nu_L}{\gamma} \qquad \gamma = 26.75 \times 10^7\ T^{-1} s^{-1}$ (for ^1H)

$$\boxed{B = 14.1\ T}$$

17.35 $\quad \nu^\circ = 200\ MHz$ and $400\ MHz$

(a) sensitivity of detection: increases b/c the larger magnetic field leads to a larger energy gap and thus a greater population in the lower-energy level.

(b) $|\delta_{CH_3} - \delta_N|$ unchanged, b/c chemical shifts do not depend on field strength.

(c) $|\nu_{CH_3} - \nu_N|$ changes, b/c Larmor frequencies do depend on field strength.

(d) J unchanged

17.36 $\quad B = 9.4\ T \qquad \nu^\circ = 400\ MHz = 400 \times 10^6\ Hz$

$$\Delta\delta = 2.5 = \delta_A - \delta_B = \left(\frac{\nu_A - \nu^\circ}{\nu^\circ} - \frac{\nu_B - \nu^\circ}{\nu^\circ}\right) \times 10^6$$

$$= \left(\frac{\nu_A}{\nu^\circ} - \frac{\nu_B}{\nu^\circ}\right) \times 10^6$$

$$= \frac{1}{\nu^\circ}(\nu_A - \nu_B) \times 10^6$$

$$= \frac{1}{400}(\nu_A - \nu_B) = 2.5$$

$$\boxed{\nu_A - \nu_B = 1000\ Hz}$$

17.37 (a) CH_3OCH_3 : one singlet

(b) $C_2H_5OC_2H_5$: one triplet and one quartet [ratio of 2:3]

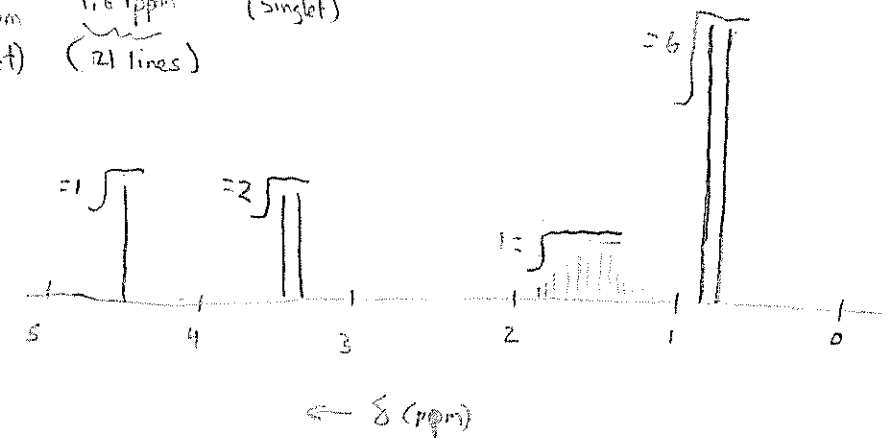
(c) C_2H_6 ; one singlet

(d) CH_3F : one doublet due to coupling w/ the $I=\frac{1}{2}$ F nucleus.

(e) $CH_3COOC_2H_5$: one singlet, one triplet, one quartet

17.38 $(CH_3)_2CHCH_2OH$

- 3.27 ppm (doublet)
- 4.50 ppm (singlet)
- 0.89 ppm (doublet)
- 1.67 ppm (21 lines)



17.39 $\nu^\circ = 60$ MHz

$B = 1.41$ T (^{1}H spectrum)

(a) $\nu_L = \frac{\gamma B}{2\pi} \Rightarrow B = \frac{2\pi\nu_L}{\gamma} = \boxed{7.05\ T}$ (Note that $B_{300} = 5B_{60}$)

(b) $\Delta\nu = \nu - \nu^\circ = \frac{\gamma}{2\pi}(B_{loc} - B'_{loc}) = \frac{\gamma}{2\pi}(\sigma^\circ - \sigma)B \qquad \Delta\nu_{60} = \frac{\gamma}{2\pi}(\sigma^\circ - \sigma)B_{60}$

$$\Delta\nu_{300} = \frac{\gamma}{2\pi}(\sigma^\circ - \sigma)B_{300} = \frac{\gamma}{2\pi}(\sigma^\circ - \sigma)(5B_{60}) = 5\Delta\nu_{60}$$

CH_3: $\Delta\nu_{300} = 5\nu_{60} = 5.140\ Hz = 700\ Hz$

aromatic: $\Delta\nu_{300} = 5.430\ Hz = 2150\ Hz$

(c) $\delta = \frac{\Delta\nu}{\nu} \times 10^6 \rightarrow$ 60 MHz: $\delta_{CH_3} = 2.3$ ppm $\delta_{aromatic} = 7.1$ ppm

300 MHz: $\delta_{CH_3} = 2.3$ ppm $\delta_{aromatic} = 7.1$ ppm

} must be the same